

Surface generating on the basis of experimental data*

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Abstract. *The problem of surface generating on the basis of experimental data is presented in this lecture. Special attention is given to the implementation of moving ordinary least squares and moving total least squares. Some results done in the Institute for Applied Mathematics in Osijek are mentioned which were published in the last several years.*

Key words: *surface generating, smoothing, moving least squares, scattered data*

Sažetak. *Generiranje ploha na osnovi eksperimentalnih podataka. U predavanju izložen je problem generiranja plohe na osnovi eksperimentalnih podataka. Kod toga posebna pažnja posvećena je primjeni pomične metode običnih i pomične metode potpunih najmanjih kvadrata. S tim u vezi navedeni su neki rezultati urađeni u Institute for Applied Mathematics in Osijek, a objavljeni u posljednjih nekoliko godina.*

Ključne riječi: *generiranje plohe, zaglađivanje, pomična metoda najmanjih kvadrata, eksperimentalni podaci*

1. Introduction

Let the data (x_i, y_i, z_i) , $i = 1, \dots, m$, be given, where $P_i(x_i, y_i) \in \Omega \subseteq \mathbb{R}^2$ are points in some region of interest, and $z_i = g(x_i, y_i) + \varepsilon_i$, where g is an unknown smooth function and $\varepsilon_i \sim N(0, \sigma^2)$. Using the given data one has to approximate the unknown function g by the function \hat{g} (global approximant).

This problem is considered by numerous authors as the global and/or local approximation or interpolation problem. Let us mention just a few of the possible applications of such problems in applied research: determining geological layers (petroleum exploration, geological maps), plotting geographical maps, investigation of heart potentials, etc. (see [3], [7], [6], [5], [14], [12], [13], [15], [20]).

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In recent literature approaches based upon least squares splines (see e.g. [10], [22]) or the one based upon moving least squares (see [4], [10], [20], [19]) are most often presented, but some other ones (see [10], [8], [6]) are presented as well.

In this lecture we shall consider the approach based on moving least squares and presented some results done at the *Institute for Applied Mathematics* in Osijek in the last several years (see [13], [14], [15], [20], [19]).

2. Moving ordinary least squares for surface generating

We are going to smooth the given data by a function \hat{g} . First, we are going to approximate the function g in a neighborhood of every point $T(\xi, \eta) \in \Omega$ in its domain by a local approximant of the form

$$\begin{aligned}\mathcal{L}^0(x, y; \mathbf{p}) &= p_1 \\ \mathcal{L}^1(x, y; \mathbf{p}) &= p_1 + p_2x + p_3y \\ \mathcal{L}^2(x, y; \mathbf{p}) &= p_1 + p_2x + p_3y + p_4xy + p_5x^2 + p_6y^2\end{aligned}\tag{1}$$

where $\mathbf{p} = (p_0, \dots, p_n)$ denotes the vector of parameters. Unknown parameters will be determined such that a more significant influence have data at points closer to the point T . In order to do this, first to each $P_i(x_i, y_i)$ we will associate a nonnegative weight function $w_i : \Omega \rightarrow [0, 1]$ which will attain its maximal value equal 1 at the point P_i and its value will die out with the distance from P_i . Various ways of choosing such weight functions can be found in the literature (see e.g. [3], [4], [10]).

Figure 1. *Weight functions*

Following [16] in the papers [13], [19] and [14] the weight function w is defined by

$$w_i(x, y) = \begin{cases} \exp\left(-\frac{1}{2\sigma_i^2}[(x - x_i)^2 + (y - y_i)^2]\right), & (x - x_i)^2 + (y - y_i)^2 \leq r_i^2 \\ 0, & (x - x_i)^2 + (y - y_i)^2 > r_i^2, \end{cases}$$

where the parameter $\sigma_i > 0$ determines the extent of the influence of the i -th data. The parameter r_i , which defines compact support of the weight function w_i is also chosen depending on σ_i .

In the paper [20] another possibility is used. As in [3], the weight function w is defined by

$$w_i(\xi, \eta) = W\left(\frac{d(P_i, T)}{\Delta_q}\right), \quad W(u) = \begin{cases} (1-u^3)^3, & 0 \leq u \leq 1, \\ 0, & u > 1. \end{cases}$$

where $d(P_i, T)$ denotes the distance from P_i to T and Δ_q is the q -th least distance $d(P_i, P_j)$, $j = 1, \dots, m$.

The optimal parameter \mathbf{p}^* for the local approximant \mathcal{L}_T in the neighbourhood of the point T can be obtained by minimizing the functional

$$F(\mathbf{p}) = \sum_{k=1}^m w_k(\xi, \eta) [\mathcal{L}_T(x_k, y_k; \mathbf{p}) - z_k]^2. \quad (2)$$

where \mathcal{L}_T is of the form (1). Minimization of the functional (2) boils down to solving the linear least squares problem

$$\mathbf{D}\mathbf{J}\mathbf{p} = \mathbf{D}\mathbf{z}, \quad (3)$$

where $\mathbf{D} = \text{diag}\left(\sqrt{w_1(\xi, \eta)}, \dots, \sqrt{w_m(\xi, \eta)}\right)$, and

$$\mathbf{J}_{ij} = \frac{\partial \mathcal{L}_T(x_i, y_i; \mathbf{p})}{\partial p_j}, \quad \mathbf{z} = (z_1, \dots, z_m)^T.$$

The most suitable method for solving the linear least squares problem (3) is the QR decomposition (see e.g. [1], [23]).

Finally, we smooth the given data (x_i, y_i, z_i) , $i = 1, \dots, m$, by the function (global approximant) \hat{g} defined by

$$\hat{g}(x, y) := \mathcal{L}_T(x, y)$$

For practical purposes, it suffices to calculate the value of the global approximant \hat{g} at finitely many points. In the papers [13] and [20] we assumed that the region of interest Ω is a rectangle $[a, b] \times [c, d]$. The local approximants were calculated on the equidistant set of nodes (ξ_i, η_j) contained in the rectangle Ω where

$$\xi_i = a + ih_x, \quad h_x = \frac{b-a}{n}, \quad \eta_j = c + jh_y, \quad h_y = \frac{d-c}{k}, \quad (4)$$

where $i = 1, \dots, n$, $j = 1, \dots, k$.

After that, the global approximant can be obtained as a least squares two-dimensional spline (see [22]). Another possibility is by following [4], to do the convex combination of the local approximants

$$\mathcal{S}(x, y) = \sum_{\nu=1}^{n \times k} \mathcal{L}_\nu(x, y) \omega_\nu(x, y), \quad \omega_\nu(x, y) = \frac{u_\nu(x, y)}{\sum_{\mu=1}^{n \times k} u_\mu(x, y)}, \quad \nu = 1, \dots, n \times k.$$

where u_ν is the weight function associated to the local approximant \mathcal{L}_ν . The weight functions u_ν can be the same as the functions w_ν , but can also be defined in another way.

In the paper [19] we are proposed an algorithm which by means of a median divides the rectangle $\Omega = [a, b] \times [c, d]$ into subcells:

$$\Omega = \bigcup_{\nu=1}^N \Omega_{\nu}, \quad \Omega_{\nu} \text{ disjoint}$$

such that each subcell Ω_{ν} contains roughly the same number of points. In each subcell we chose only one node. Namely, the local approximants would then be located at the neighbourhood of the centroid $(\bar{\xi}_{\nu}, \bar{\eta}_{\nu})$ of the subcell Ω_{ν} , where $\bar{\xi}_{\nu}$ (resp. $\bar{\eta}_{\nu}$) represents the arithmetic mean of all x_i (resp. y_i), whose corresponding data points lie in the subcell Ω_{ν} (see *Fig. 1.*). The centroid $(\bar{\xi}_{\nu}, \bar{\eta}_{\nu})$ has a property that the sum of squared distances to all data points in that subcell is minimal ([3]). The number of data points in the subcell should be sufficient for evaluating parameters of the local approximant. By evaluation of the local approximant for the centroid $(\bar{\xi}_{\nu}, \bar{\eta}_{\nu})$ the data used in evaluating this local approximant would be taken from a somewhat larger region containing Ω_{ν} .

In that way the number of nodes at which we evaluate local approximants can be considerably reduced, and local approximants can be chosen in the class of the quadratic function of two variables (local paraboloids).

Remark 1. *In literature there also appear other method of choosing the allocation of nodes at which we evaluate local approximants. It would be more acceptable to use polygons for the shape of a subcell in the partition of the basic cell. In that case the Dirichlet or Delaunay tessellation (see e.g. [2]) should be used.*

The optimal allocation of nodes is according to ([4]) attained at the global minimum of the function:

$$GN^2 = \sum_{i=1}^m \min_{\nu} [(x_i - \bar{\xi}_{\nu})^2 + (y_i - \bar{\eta}_{\nu})^2],$$

and the measure of the “equal representation” is given by $D = \sum_{\nu=1}^N (q_{\nu} - \frac{m}{N})^2$, where q_{ν} is the number of data points in the ν -th subcell.

3. Moving total least squares for surface generating

When the errors occur in measurements of all the variables, it makes more sense to determine the local approximants in the sense of the *total least squares* (see e.g. [1], [9], [11], [17], [16]). We are going to call this method the **moving total least squares method** (MTLS method). In this sense in the papers [15] and [20] we suppose that

$$z_i = g(\mathbf{x}_i + \delta_i) + \varepsilon_i, \quad i = 1, \dots, m,$$

where ε_i denotes the unknown error in z_i , and δ_i is the vector of unknown errors in \mathbf{x}_i . Furthermore, we suppose that ε_i is a normal random variable with mean 0 and variance σ^2 , and δ_i are normal random vectors with mean $\mathbf{0}$ and the covariance matrix $\sigma^2 \mathbf{I}$.

In the neighbourhood of the point $T(\xi, \eta)$ we are going to approximate the function g by a *local total least squares plane*. Since this local plane always goes through the weighted centroid of the data (see [20]), we shall search for it of the form

$$r_T(\xi - \bar{\xi}_T) + s_T(\eta - \bar{\eta}_T) + t_T(\zeta - \bar{\zeta}_T) = 0,$$

where

$$\bar{\xi}_T := \frac{1}{\kappa_T} \sum_{i=1}^m w_i(\xi, \eta) x_i, \quad \bar{\eta}_T := \frac{1}{\kappa_T} \sum_{i=1}^m w_i(\xi, \eta) y_i, \quad \bar{\zeta}_T := \frac{1}{\kappa_T} \sum_{i=1}^m w_i(\xi, \eta) z_i,$$

with $\kappa_T := \sum_{i=1}^m w_i(\xi, \eta)$. The optimal parameters r_T^*, s_T^*, t_T^* of the local TLS plane are obtained by minimization of the functional

$$G(r_T, s_T, t_T) = \sum_{i=1}^m w_i(\xi, \eta) \frac{[r_T(x_i - \bar{\xi}_T) + s_T(y_i - \bar{\eta}_T) + t_T(z_i - \bar{\zeta}_T)]^2}{r_T^2 + s_T^2 + t_T^2} \quad (5)$$

The minimum of the functional G is attained at the eigenvector corresponding to the smallest eigenvalue of the matrix $\mathbf{B}^T \mathbf{B}$, where

$$\mathbf{B} := \begin{bmatrix} \sqrt{w_1(\xi, \eta)}(x_1 - \bar{\xi}_T) & \sqrt{w_1(\xi, \eta)}(y_1 - \bar{\eta}_T) & \sqrt{w_1(\xi, \eta)}(z_1 - \bar{\zeta}_T) \\ \vdots & \vdots & \vdots \\ \sqrt{w_m(\xi, \eta)}(x_m - \bar{\xi}_T) & \sqrt{w_m(\xi, \eta)}(y_m - \bar{\eta}_T) & \sqrt{w_m(\xi, \eta)}(z_m - \bar{\zeta}_T) \end{bmatrix}$$

(see [11], [20]).

Thus, if the third component of the eigenvector corresponding to the smallest eigenvalue of the matrix $\mathbf{B}^T \mathbf{B}$ is non-zero, the local TLS plane in the neighbourhood of the point (ξ, η) is defined by (see [20]):

$$\mathcal{L}_T(\xi, \eta) = \begin{cases} -\frac{r_T^*}{t_T^*}(\xi - \bar{\xi}_T) - \frac{s_T^*}{t_T^*}(\eta - \bar{\eta}_T) + \bar{\zeta}_T & , t_T^* \neq 0 \\ \bar{\zeta}_T & , t_T^* = 0 \end{cases} \quad (6)$$

The TLS local plane will be determined on the net of nodes defined by (4). Finding an eigenvector corresponding to the smallest eigenvalue of the regular matrix $\mathbf{B}^T \mathbf{B}$ can be made very efficient because of the particular form of this matrix (see [21]). First, take the QR -decomposition of the matrix \mathbf{B} , by which the matrix $\mathbf{B}^T \mathbf{B}$ becomes

$$\mathbf{B}^T \mathbf{B} = \mathbf{R}^T \mathbf{R},$$

where \mathbf{R}^T is a lower-triangular and \mathbf{R} is an upper-triangular matrix. Now, by using the *Inverse Power Method* we easily obtain an eigenvector corresponding to the smallest eigenvalue of the matrix $\mathbf{R}^T \mathbf{R}$. The rate of convergence of the Inverse Power Method is linear, but with a good choice of the initial vector, the convergence can be quite fast. Therefore, at each node (ξ_i, η_j) we take for the initial vector the vector obtained earlier for the previous node. Doing so, the number of iterations in the Inverse Power Method needed at each node is small (usually 1–2, seldom 3–4). Note, moreover, that the matrix used at each iteration step is the same.

4. Numerical examples

Example 1. Consider the function $g(x, y) = (x^2 - y^2)^2$ defined on the region $\Omega = [-1, 1] \times [-1, 1]$. Take a random uniformly distributed set of points $P_i(x_i, y_i)$, $i = 1, \dots, 225$, in Ω (see Fig. 3 and take $z_i := g(x_i + \delta_i^x, y_i + \delta_i^y) + \varepsilon_i$, $i = 1, \dots, m$, where $\delta_i^x \sim N(0, 0.07)$, $\delta_i^y \sim N(0, 0.07)$ and $\varepsilon_i \sim N(0, 0.05)$.

Fig. 2a shows the graph of the function g , and Fig. 2b shows the data surface using the Delaunay tessellation.

a) Graph of the function g

b) Generated data

Figure 2. Graph of the function g and the generated data

If the rectangle Ω according to the algorithm proposed in [19] is divided into subcells such that each subcell contains roughly 18 data points, we obtain 16 subcells. Fig. 3 shows the data points, subcells and the corresponding centroids. Fig. 4.a shows the corresponding surface obtained as a convex combination of the local paraboloids generated in centroids of subcells.

a) Data points

b) Choice of nodes

Figure 3. Data points and the choice of nodes

The same surface is generated by using moving total least squares as proposed in [20]. For that purpose the nodes (ξ_i, η_j) in the region Ω are determined by $h_x =$

$h_y = 0.2$, and each TLS local plane is determined by using $q = 15$ nearest neighbour points.

Fig. 4b shows the graph of the approximation \hat{g} of the function g , which was obtained as a convex combination of local TLS planes.

- | | |
|---|--|
| <p>a) Convex combination
of the local paraboloids</p> | <p>b) Convex combination
of local TLS planes</p> |
|---|--|

Figure 4. Generated surfaces

Example 2. Along the the skin of the back fat of the pig the thickness is measured by ultrasound every 14 days at about 20 points on the right half of the pig. On the basis of these measurements a surface is generated which shows the configuration and thickness of back fat of the measured pig. We shall use the moving total least squares method described in ([20]). In surface generating it is taken into consideration that errors can appear both in the measured thickness of back fat and in the coordinates of the point at which the measurement was done. Fig. 5 shows a such generated surface.

- | | |
|---|---|
| <p>a) Surface of pig's
back fat</p> | <p>b) cross-sections along
the spine of the pig</p> |
|---|---|

Figure 5. Surface of pig's back fat and cross-sections along the spine of the pig

Cross-sections along the spine of the pig done during measurement can also be seen in Fig. 5. This investigation was used for decision making in pigs-selection.

References

- [1] A. BJÖRCK, *Numerical Methods for Least Squares Problems*, SIAM, Philadelphia, 1996
- [2] A. BOWYER, *Computing Dirichlet tessellation*, Computer Journal **24**(1981) 162–166
- [3] W. S. CLEVELAND, S. J. DEVLIN, AND E. GROSE, *Regression by local fitting: Methods, properties, and computational algorithms*, Journal of Econometrics **37**(1988) 87–114
- [4] R. FARWIG, *Multivariate interpolation of scattered data by moving least squares methods*, in: Algorithms for Approximation, (J. C. Mason and M. G. Cox, Eds.), Clarendon Press, Oxford, 1987, pp. 193–211.
- [5] R. FRANKE, K. ŠALKAUŠKAS, *Localization of multivariate interpolation and smoothing methods*, J. Comput. Appl. Math. **73**(1996) 79–94
- [6] R. FRANKE, H. HAGEN, *Least squares surface approximation to scattered data using multiquadratic functions*, Advances in Computational Mathematics **2**(1994) 81–99
- [7] R. FRANKE, *Scattered data interpolation: Test of some methods*, Math. Comp. **38**(1982) 99–106
- [8] H. HAGEN, *Topics in Surface Modelling*, SIAM, Philadelphia, 1992.
- [9] S. VAN HUFFEL, J. VANDEWALLE, *The Total Least squares Problem: Computation Aspects and Analysis*, Frontiers in Appl. Math. Ser., Vol. 9., SIAM, Philadelphia, 1991.
- [10] P. LANCASTER, K. SALKAUŠKAS, *Curve and Surface Fitting: An Introduction*, Academic Press, London, 1986.
- [11] Y. NEIVERGELT, *Total least squares: State-of-the-art regression in numerical analysis*, SIAM Review **36**(1994) 258–264
- [12] L. SCHUMAKER, *Fitting surfaces to scattered data*, in Approximation Theory II, (G. G. Lorenz, C. K. Chui, and L. Schumaker, Eds.), Academic Press, New York, 1976.

- [13] R. SCITOVSKI, D. JUKIĆ, I. BAŠIĆ, *Application of the moving least squares method in surface generating*, in: Proceedings of 17th Int. Conf. Information Technology Interfaces, (D. Kalpić, V. Hljuz-Dobrić, Eds.), Zagreb, 1995, 461–467.
- [14] R. SCITOVSKI, R. GALIĆ, I. KOLUND, I. BAŠIĆ, D. JUKIĆ, *Procjena rasprostriranja slojeva tla po dubini sondažnog profila*, u: T. Hunjak, Lj. Martić, L. Neralić, Zbornik radova KOI'95, Zagreb, 1995, 111–120.
- [15] R. SCITOVSKI, Š. UNGAR, D. JUKIĆ, M. CRNJAC, *Moving total least squares for parameter identification in mathematical model*, in Operations Research Proceedings 1995, (P. Kleinschmidt et al., Eds.) Springer-Verlag, Berlin, 1996, 196–201.
- [16] R. SCITOVSKI, D. JUKIĆ, *A method for solving the parameter identification problem for ordinary differential equations of the second order*, Applied Mathematics and Computation **74**(1996) 273–291
- [17] R. SCITOVSKI, D. JUKIĆ, *Total least squares problem for exponential function*, Inverse Problems - An International Journal of Inverse Problems, Inverse Methods and Computerized Inversion of Data **12**(1996) 341–349
- [18] R. SCITOVSKI, *Analysis of parameter identification problem*, Applied Mathematics and Computation, **82**(1997) 39–55
- [19] R. SCITOVSKI, R. ŠALIĆ, K. PETRIĆ, K. SABO, *Optimal allocation of nodes for surface generating*, in: Proceedings of 19th Int. Conf. Information Technology Interfaces, (D. Kalpić, V. Hljuz-Dobrić, Eds.), Zagreb, 1997, 461–467.
- [20] R. SCITOVSKI, Š. UNGAR, D. JUKIĆ, *Approximating surface by moving total least squares method*, to appear
- [21] I. SLAPNIČAR, *Accurate computation of singular values and eigenvalues of symmetric matrices*, Mathematical Communications **1**(1996) 153–167
- [22] H. SPÄTH, *Spline-Algorithmen zur Konstruktion glatter Kurven und Flächen*, R. Oldenbourg Verlag, München, 1973
- [23] L. N. TREFETHEN, D. BAU, III, *Numerical Linear Algebra*, SIAM, Philadelphia, 1997.